AD-A162 785 PROJECT: SUBMICRON PHONONICS I 1 THE PROBLEMATICS OF PHONON DISTURBANCES IN DC SEMICONDUCTOR TRANSPORT(U) GRAZ UNIV (AUSTRIA) P KOCEVAR OCT 85 DAJA45-84-M-0304 1/1

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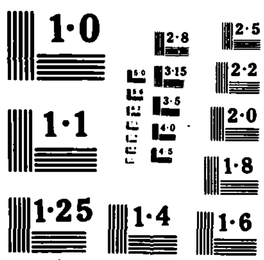
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FINAL REPORT
(Contract Nr. DAJA45-84-M-0394)

(1)

Project: SUBMICRON PHONONICS I

1. The Problematics of Phonon Disturbances in d.c. Semiconductor Transport

Since the early days of modern solid-state theory phonon disturbances have been discussed in connection with fundamental aspects of charge transport. Peierls (1930) and later Klemens (1951) had recognized their importance and particularly the essential role of nonelectronic relaxation processes of the nonequilibrium phonons for the establishment of a steady state of the coupled carrier-phonon system in the presence of a d.c. electric field. Contributions of mutual drag effects between carriers and phonons to the electrical and thermal conductivity and to the thermopower of semiconductors were first estimated by Sondheimer and Parrot (1956,1957), who also pointed out, that the neglect of phonon disturbances in the calculation of electronic transport coefficients leads to violation of the Onsager and Kelvin relations. It is interesting to note, that even in the ohmic case, any drag-effect of nonequilibrium phonons on the electronic mobility introduces a nonlinear electronic response, because the phonon-distributions and therefore the rates for carrier-phonon scattering become field dependent, in contrast to the linear-response concept of field independent electronic mobilities. But the most practical aspects of phonon disturbances have arisen in connection with the nonlinear response phenomena connected with high field transport and high optical excitation of semiconductors.

Because of the rapid increase of the thermalization rate of acoustic modes with temperature, possible mobility effects of acoustic phonon disturbances are restricted to lattice temperatures of at most a few degrees K. At these temperatures the great uncertainties in the treatment of the dominant ionized impurity scattering overshadow any nonequilibrium phonon effects on the theoretical carrier mobilities.

In contrast to the acoustic case, the thermalization rates of optical phonons are weakly temperature dependent. Although these rates are very fast, of the order of 10^{12} sec^{-1}, the strong polar optical carrier-LO-phonon coupling in polar

materials can lead to even faster emission rates of phonons by the carriers and therefore to substantial LO-phonon amplification even at room-temperature.

The practically most interesting candidate among the standard semiconductor materials for noticeable mobility-effects of such nonequilibrium LO-phonons is n-GaAs, because the time-constants for valley-transfer, again in the psec-range, are comparable to the above discussed time constants for the build-up of phonon disturbances. Since the phonon amplification will in turn modify the carrier distributions, there might be possible interference effects between the phonon build-up and the performance of high speed GaAs devices laid out to work in the psec regime.

The present research project was set up to provide a first step towards a quantitative theory of such transient nonequilibrium phonon effects in GaAs devices.

2. Scope and Objectives of the Project

The main objectives of the present project were:

(A) to develop a FORTRAN-code for distribution functions of nonequilibrium phonons to be used in heated displaced maxwellian (HDM) models of nonlinear transport in GaAs-devices, with the purpose to provide semi-quantitative calculations of nonequilibrium phonon effects on the electronic properties of small devices;

(B) to determine the magnitude of such effects;

(C) to determine feasibility and value of a major effort to integrate highly accurate phonon-electron effects into a more precise electron-transport code.

3. Results

3A (regarding item 2A):

The FORTRAN-code for the standard-band model of GaAs, whose flow-chart was presented in the second interim report for this project, has been extended to include, within the HDM-approach, the intervalley scattering of electrons between the central Γ-valley and the four secondary L-valleys. Particle, energy and momentum transfers were taken from the HDM-theory of Butcher and Fawcett (Proc. Phys. Soc. 86, 1205 (1965)).

The code was organized in such a way, as to match the stepwise time-integration of Dr.Grubin's HDM-model for space-dependent transport, inferred from his recent publications in VLSI Electronics: Microstructure Science, Vol.3, p.197 (1982) and Vol.10, p.237 (1985).

Physical ingredients:

1. Neglect of any LO-phonon diffusion during the psec time regime of the transient valley-transfer and nonequilibrium phonon effects, justified by the very small dispersion and resulting negligible propagation velocity of long-wavelength optical phonons. The subroutine SUMBAL provides the instantaneous phonon distributions for each coarse-grained-space cell.
2. At each time-step, the Grubin-code, during its search for the new carrier parameters $v_d(\Gamma)$, $v_d(L)$, $T_c(\Gamma)$, $T_c(L)$, $n_c(\Gamma)$ and $n_c(L)$ asks SUMBAL for the phonon distributions $N_{LO}, \ldots$, corresponding to the momentary trial-values of the parameters. The phonon distributions can be printed out as functions of their wavevector $\vec{q}$. SUMBAL also contains the possibility to provide instantaneous carrier-concentrations for the case of an "adiabatic"adaption of the carriers to the momentary phonon distributions. For this "adiabatic approximation" SUMBAL also calculates the contributions of all scattering mechanisms to the total energy and momentum balance per cm^{-3} (SUMmation of BALance contributions).

3. Inclusion of the following carrier-scattering mechanisms (i) ionized impurity scattering, (ii) acoustic deformation potential scattering to LA-acoustic phonons,(iii) piezoelectric scattering to LA and TA-acoustic phonons.
4. Optional inclusion of acoustic phonon disturbances (for eventual use in low-temperature, c.w.-pulse situations).
5. Use of the most recent experimentally determined thermalization rates for all phonon-modes with the exception of the intervalley phonons, for which no experimental evidence of electronically induced perturbations have been found in recent laser-excitation experiments, so that they are assumed to be unperturbed, i.e. having infinite thermalization rates.

Technical details:

The full code for the "adiabatic model", containing the subroutine SUMBAL to be used in Dr.Grubin's calculations, are available on tape and as listing of the program. Due to our complete ignorance of both Dr.Grubins computer-code and machine-system, the technicalities of the installation of SUMBAL will have to be guided by Dr.Grubin.

3B (regarding item 2B):

As estimate of possible effects of LO-phonon amplification on the electronic mobility of GaAs, the following "adiabatic", single-valley transport model was set up,providing also the simplest test of our nonequilibrium phonon code (see list of publications Nr.1):

The time-integration of the phonon Boltzmann equations is performed in parallel to the solution of the number, energy, and momentum balances for the carriers in the Γ and L-valleys. This procedure is possible, because the high carrier concentrations and carrier-carrier scattering rates imply a very rapid adaption of the HDM distribution to any change in the phonon populations. Of course the "adiabaticity" of the carriers also requires, that the carriers are completely "slaved" by the phonons, since the whole time-dependence of the coupled carrier-phonon system only arises from the phonon-dynamics, while at each time-instant the density, energy and momentum of the carriers are assumed to be balanced like in a conventional steady-state calculation. This would be fully justified only, if all dominant time-constants for the carrier-dynamics were much smaller than the total relaxation time in the phonon Boltzmann equation. While this requirement is reasonably well fulfilled for the polar optical interaction, the valley-transfer rate of the carriers is comparable to the amplification-rate of the LO-phonons. So the inclusion of intervalley transfer introduces a competing time-scale, so that the justification of the adiabatic model is much less satisfactory than for the single-valley case.

So the installation of SUMBAL into Dr.Grubin's code for a parallel time-integration of the carrier-numbers, energies and momenta will allow to treat all time-variations in the problem in parallel, with no need of carrier-slavery by the phonons. Moreover, our explorative results for the "adiabatic" single-valley model of GaAs demonstrate the necessity for such a full time-analysis. Figures 1,2,3 show, that the intra - valley carrier-phonon dynamics in itself leads to non equilibrium *LO-phonon induced breakdown effects of the Fröhlich-Paranjape* type for fields, carrier-concentrations and time-intervals typical for the appearance of valley-transfer and velocity-overshoot in the usual many valley models for phonon equilibrium (see list of publications Nr.1). Whether or not such a breakdown of the (locally) homogeneous HDM-transport will occur in the realistic many valley model will have to be investigated with Dr.Grubin's more elaborate and time-consuming computer-codes.

3C (referring to 2C):

In view of the strong dependence of the intravalley breakdown on a sufficient density of carriers in the valley, the still

unknown interplay between intervalley transfer and the phonon effects do not allow to rule out similar breakdown phenomena for the many-valley case.

Moreover, since Fröhlich-type breakdown within the rather restrictive HDM-framework only implies the breakdown of the model and not necessarily of the locally homogeneous charge-transport in n-GaAs, we plan not only to extend our "adiabatic code" to a better treatment of the time-evolution, but have recently set-up a research project of including nonequilibrium phonons into Monte-Carlo-codes of hot carriers (see list of publications Nr.2). In any case it is obvious, that including phonon-disturbances in the highly sophisticated space-and time-analysis based on Dr.Grubin's HDM-approach will, as in many similar cases of the use of the HDM-model, give the first and, moreover, even a *semiquantitative picture of a hitherto* unexplored and controversial effect.

4. Publications

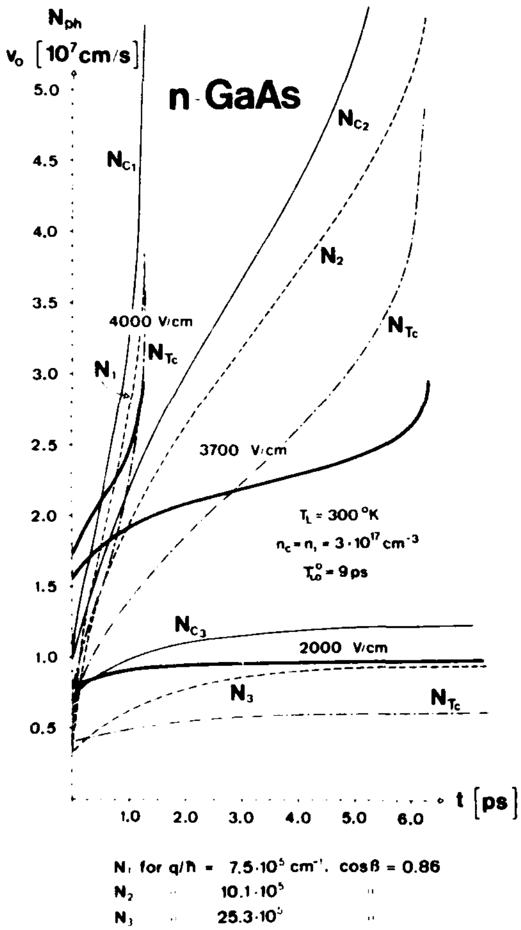
1. P.Kocevar: "Hot Phonon Dynamics", invited paper at the 4th Int. Conference on Hot Electrons in Semiconductors (Innsbruck, 1985), Physica B, in print.
2. P.Bordone, C.Jacoboni, P.Lugli, L.Reggiani, and P.Kocevar: "Monte Carlo Analysis of Hot-Phonon Effects in Semiconductor Transport Properties", ibid.

5. List of Participating Scientific Personnel

P.Kocevar (Inst.f.Theor. Physik, Univ.Graz, Austria)
E.Waupot (" " " ")

P. Kocevar

October 1985 (Dr.P.Kocevar)



Time Evolution of Mean Driftvelocity, Carrier Temperature, and LO-Phonon Distributions for Single Valley Model.

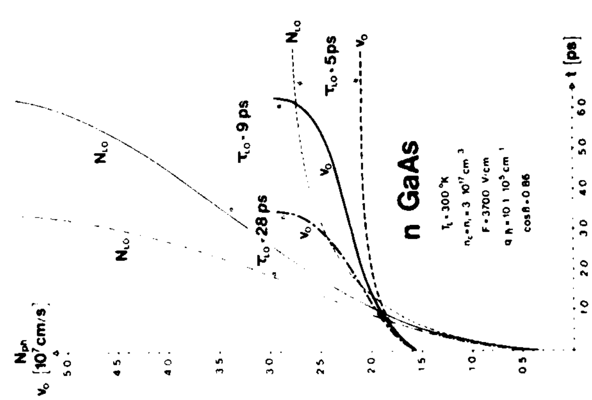


FIGURE 3: Dependence of Intravalley Breakdown on LO-Phonon Lifetime

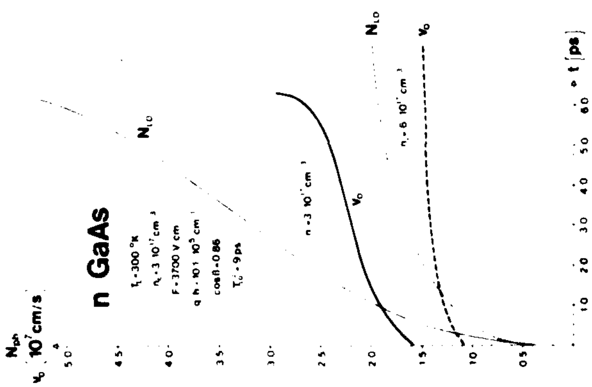


FIGURE 4: Dependence of Intravalley Breakdown on Compensation

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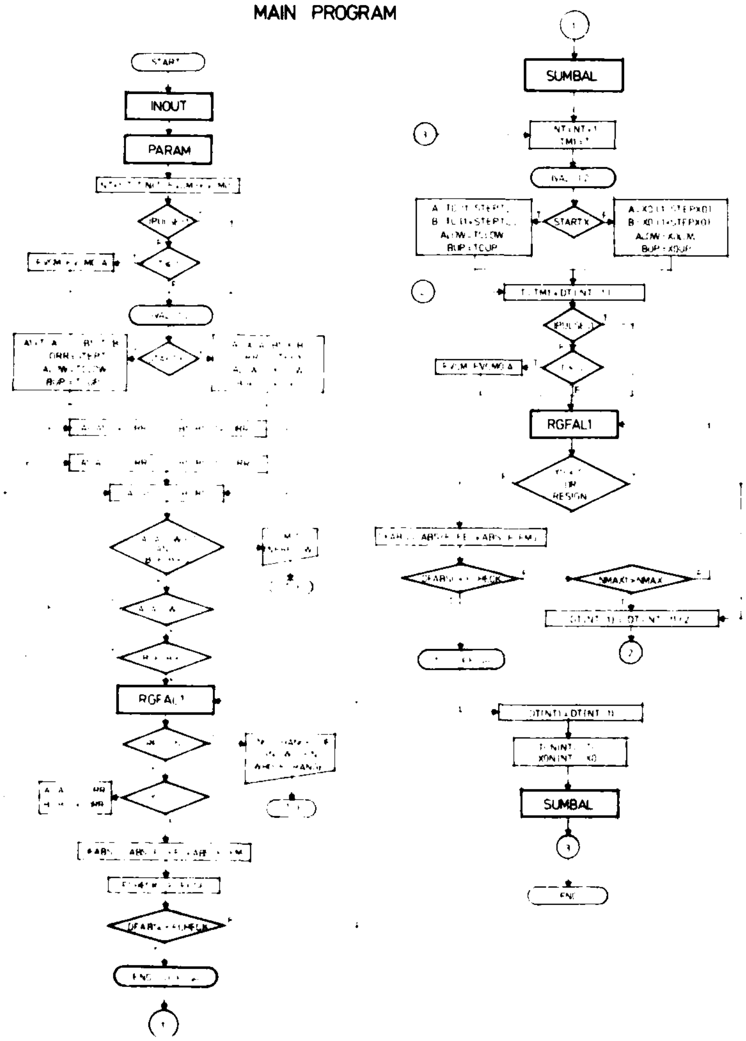
MAIN PROGRAM



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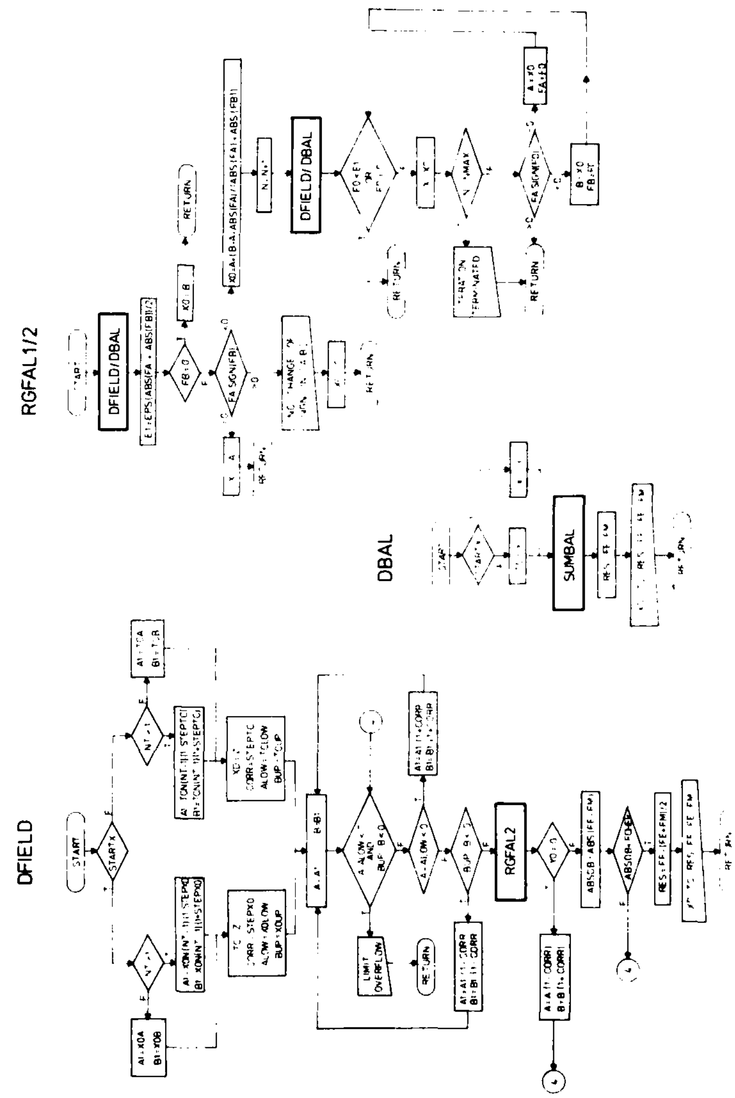
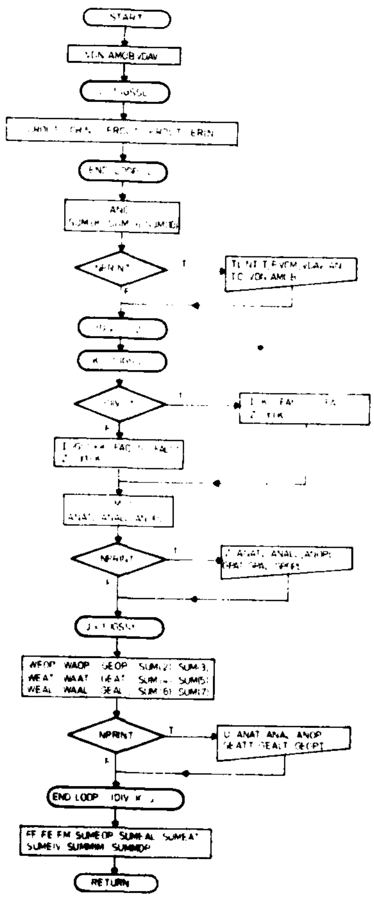


FLOW-CHART

SUMBAL



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